Montes Taurus J. Pure Appl. Math.
2 (1), 1-8, 2020

TOPOLOGICAL INDICES OF DOPAMINE

AYSUN YURTTAS GUNES*

Abstract. In the last seven decades, there has been an increasing interest in topological graph indices due to their practical applications in many areas of science including chemistry, pharmacology, physics and biology. These indices are mathematical formulae which help one to calculate some number which predicts some physical or chemical properties of the chemical molecules under investigation. In this paper, we investigate some topological graph indices in relation with the organic chemical compound called dopamine which plays an important role in brain and body.
Keywords: Graph, dopamine, Zagreb indices, topological indices.
MSC(2010): 05C10, 05C30, 68R10, 68Uxx.

1. Introduction

Dopamine (DA, a contraction of 3,4-dihydroxyphenethylamine), see Figure 1, is an organic chemical of the catecholamine together with phenethylamine families that plays several very important roles in the brain and body.

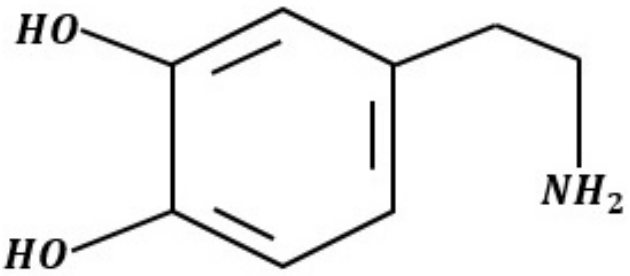

Figure 1. Dopamine

It is an amine which is synthesized by removing a carboxyl group from a molecule of its precursor chemical L-DOPA, synthesized in the brain and kidneys. Dopamine is also synthesized in plants and most animals. In the

Date: Received: 12 December 2019, Accepted: 10 February 2020.
*Corresponding author.

© Montes Taurus Journal of Pure and Applied Mathematics (MTJPAM)

brain, dopamine functions as a neurotransmitter a chemical released by neurons (nerve cells) to send signals to other neurons. The brain includes several distinct dopamine channels and one of them plays an important role in the motivational component of reward-oriented behaviour. The anticipation of most of the types of rewards increases the amount of dopamine in the brain and many addictive drugs increase dopamine release or block its reuptake into neurons following its release. Other brain dopamine channels are involved in the motor control and in the control of the release of various hormones. These channels and cell groups form a dopamine system which acts as neuro-modulatory. Several important diseases of the neural system are associated with dis-function of the dopamine system, and some of the key medications used to treat these problems work by altering the effects of dopamine.

In popular culture and media, dopamine is often seen as the main chemical causing pleasure, but the current opinion in pharmacology is that dopamine instead affects incentive salience, meaning that it signals the value of an outcome which motivates the organism to achieve an outcome.

Dopamine was first synthesized in 1910 by Barger and Ewens at Wellcome Laboratories in London, [1], and first identified in the human brain by Montagu in 1957. It was named dopamine because it is a monoamine whose precursor in the Barger-Ewens synthesis is 3,4-dihydroxyphenylalanine (levodopa or L-DOPA). Dopamine's function as a neurotransmitter was first recognized in 1958 by Carlsson and Hillarp at the Laboratory for Chemical Pharmacology of the National Heart Institute, [2].

A dopamine molecule has a catechol structure (a benzene ring with two hydroxyl side groups) with one amine group attached via an ethyl chain. As such, dopamine is the simplest possible catecholamine, a family that also includes the neurotransmitters norepinephrine and epinephrine. The existence of a benzene ring in this amine attachment makes it a substituted phenethylamine, a family including some of the psychoactive drugs.

Topological graph indices are defined and used in many fields to study several properties of different objects including atoms and molecules. A large number of topological graph indices have been defined and studied by many mathematicians and chemists as most graphs are generated from molecules by replacing atoms with vertices and bonds with edges. They are defined as topological graph invariants measuring several physical, chemical, pharmacological, pharmaceutical, biological, etc. properties of graphs modelling real life situations. They can be grouped into three classes according to the way of definition: by vertex degrees, by matrices or by distances.

Let $G = (V, E)$ be a simple graph with $\mid V(G) \mid = n$ vertices and $\mid E(G) \mid = m$ edges. That is, we do not allow loops or multiple edges. For a vertex $v \in V(G)$, we denote the degree of v by $d_G(v)$ or d_v.

Two of the most frequently used topological graph indices are known as the first and second Zagreb indices respectively denoted by $M_1(G)$ and $M_2(G)$:

$$M_1(G) = \sum_{u \in V(G)} d_G^2(u) \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v). \tag{1.1}$$

They were defined in 1972 by Gutman and Trinajstic, [3], and are often referred to due to their uses in QSAR and QSPR studies in molecular chemistry. In [5], some results on the first Zagreb index together with some other indices are given. For some graph operations, these indices are calculated in [6].

The F-index or with its commonly referred name, forgotten index of a graph G is denoted by $F(G)$ or $M_3(G)$ and is defined as the sum of the cubes of the degrees of the vertices of the graph. The total π-electron energy of a graph depends on the degree based sums $M_1(G)$ and $F(G) = \sum_{u \in V(G)} d_G^3(u)$. They were first appeared in the study of structure-dependency of total π-electron energy in 1972, [11]. The first index was later named as the first Zagreb index and the second sum has never been further studied. As a result, this sum was recently named the forgotten index or the F-index by Furtula and Gutman, [8], and it was shown to have an exceptional applicative potential.

The hyper-Zagreb index is similarly defined in [8] as a variety of the classical Zagreb indices as

$$HM(G) = \sum_{(uv \in E} (d_u + d_v)^2.$$

Inspired by the study of heat formation in heptanes and octanes in [13], Furtula et. al. proposed an index, called the Augmented Zagreb index, which predicts better. It is defined by

$$AZI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v - 2}.$$

The Harmonic index was introduced by Zhong, [9], who found that it correlates well with Π-electron energy of benzenoid hydrocarbons and defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

Ranjini et al., [7], re-defined the existing Zagreb indices and named them the redefined first, second and third Zagreb indices for a graph G and they respectively are

$$ReZG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \cdot d_v}, \qquad ReZG_2(G) = \sum_{uv \in E(G)} \frac{d_u \cdot d_v}{d_u + d_v},$$

and

$$ReZG_3(G) = \sum_{uv \in E(G)} (d_u \cdot d_v)(d_u + d_v).$$

Milicevic et. al., [10], reformulated the Zagreb indices in terms of the edge degrees instead of the vertex-degrees as

$$RM_1(G) = \sum_{uv \in E(G)} d(uv)^2, \quad \text{and} \quad RM_2(G) = \sum_{e,e' \in E(G)} d(e)d(e').$$

Aram and Dehgardi, [4], introduced the concept of reformulated F-index as

$$RF(G) = \sum_{uv \in E(G)} d(uv)^3.$$

Kulli, [12], introduced the first and second Banhatti indices, intending to take into account the contributions of pairs of incident elements. They are defined as

$$B_1(G) = \sum_{u,e} [d_G(u) + d(e)], \quad \text{and} \quad B_2(G) = \sum_{u,e} d_G(u)d(e).$$

Naji et. al. elaborated the idea of using the second degree of a vertex, $d_2(u)$, namely the number of second neighbors. This leads to three leap Zagreb indices defined by

$$LM_1(G) = \sum_{u \in V(G)} d_2(u)^2, \qquad LM_2(G) = \sum_{uv \in E(G)} d_2(u)d_2(v),$$

and

$$LM_3(G) = \sum_{u \in V(G)} d(u)d_2(u).$$

2. Main Results

Now we will determine some well-known topological indices of dopamine:

Theorem 2.1. *The first and second Zagreb indices of dopamine are* $M_1(G) = 50$ *and* $M_2(G) = 46$.

Proof. We partition the edges of dopamine $C_8H_{11}NO_2$ into edges of the type $E_{(d_u,d_v)}$ where uv is an edge. In $C_8H_{11}NO_2$, we get edges of the type $E_{(1,2)}, E_{(1,3)}, E_{(2,2)}, E_{(2,3)}$ and $E_{(3,3)}$. The number of edges of these types are 1, 2, 2, 5 and 1, respectively.

We know that $M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$, i.e.,

$$\begin{aligned} M_1(C_8H_{11}NO_2) &= \mid E_{(1,2)} \mid (1+2) + \mid E_{(1,3)} \mid (1+3) + \mid E_{(2,2)} \mid (2+2) \\ &+ \mid E_{(2,3)} \mid (2+3) + \mid E_{(3,3)} \mid (3+3) \\ &= 1(1+2) + 2(1+3) + 2(2+2) + 5(2+3) + 1(3+3) = 50. \end{aligned}$$

As $M_2(G) = \sum_{uv \in E(G)} d_u d_v$, we get the result by similar calculations. □

Theorem 2.2. *The third Zagreb index (forgotten index) of dopamine is* $F(G) = 124$.

Proof. Recall that $F(G) = \sum_{u \in V(G)} {d_u}^3$implying that

$$F(C_8H_{11}NO_2) = \sum_{u \in V(C_8H_{11}NO_2)} {d_u}^3 = 1^3 \cdot 3 + 2^3 \cdot 5 + 3^3 \cdot 3 = 124.$$

□

Theorem 2.3. *The hyper-Zagreb index of dopamine is* $HM(C_8H_{11}NO_2) = 234$.

Proof. We know that $HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2$, i.e.,

$$\begin{aligned} HM(C_8H_{11}NO_2) &= \mid E_{(1,2)} \mid (1+2)^2 + \mid E_{(1,3)} \mid (1+3)^2 + \mid E_{(2,2)} \mid (2+2)^2 \\ &+ \mid E_{(3,2)} \mid (3+2)^2 + \mid E_{(3,3)} \mid (3+3)^2 \\ &= 1(1+2)^2 + 2(1+3)^2 + 2(2+2)^2 + 5(3+2)^2 + 1(3+3)^2 \\ &= 9 + 32 + 32 + 125 + 36 = 234. \end{aligned}$$

□

Theorem 2.4. *The augmented Zagreb index of dopamine is* $AZI(C_8H_{11}NO_2) = 82,14$.

Proof. We know that $AZI(G) = \sum_{uv \in E(G)} (\frac{d_u \cdot d_v}{d_u + d_v - 2})^3$. Hence

$$\begin{aligned} AZI(C_8H_{11}NO_2) &= \mid E_{(1,2)} \mid (\frac{1 \cdot 2}{1+2-2})^3 + \mid E_{(1,3)} \mid (\frac{1 \cdot 3}{1+3-2})^3 + \\ \mid E_{(2,2)} \mid (\frac{2 \cdot 2}{2+2-2})^3 &+ \mid E_{(2,3)} \mid (\frac{2 \cdot 3}{2+3-2})^3 + \\ \mid E_{(3,3)} \mid (\frac{3 \cdot 3}{3+3-2})^3 &= 1 \cdot 2^3 + 2(\frac{3}{2})^3 + 2 \cdot 2^3 + 5 \cdot 2^3 + 1(\frac{9}{4})^3 = 82,14. \end{aligned}$$

□

Theorem 2.5. *The harmonic index of dopamine is* $H(C_8H_{11}NO_2) = 5$.

Proof. We know that $H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$, i.e.,

$$\begin{aligned} H(C_8H_{11}NO_2) &= \mid E_{(1,2)} \mid \frac{2}{1+2} + \mid E_{(1,3)} \mid \frac{2}{1+3} + \mid E_{(2,2)} \mid \frac{2}{2+2} \\ &+ \mid E_{(2,3)} \mid \frac{2}{2+3} + \mid E_{(3,3)} \mid \frac{2}{3+3} \\ &= 1 \cdot \frac{2}{3} + 2 \cdot \frac{2}{4} + 2 \cdot \frac{2}{4} + 5 \cdot \frac{2}{5} + 1 \cdot \frac{2}{6} = 5. \end{aligned}$$

□

Theorem 2.6. *The re-defined versions of Zagreb indices of dopamine are* $ReZG_1(C_8H_{11}NO_2) = 11$, $ReZG_2(C_8H_{11}NO_2) = \frac{70}{6}$, $ReZG_3(C_8H_{11}NO_2) = 266$.

Proof. We know that $ReZG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \cdot d_v}$, i.e.,

$$\begin{aligned} ReZG_1(C_8H_{11}NO_2) &= \mid E_{(1,2)} \mid \frac{1+2}{1\cdot 2} + \mid E_{(1,3)} \mid \frac{1+3}{1\cdot 3} + \mid E_{(2,2)} \mid \frac{2+2}{2\cdot 2} \\ &+ \mid E_{(2,3)} \mid \frac{2+3}{2\cdot 3} + \mid E_{(3,3)} \mid \frac{3+3}{3\cdot 3} \\ &= 1\cdot\frac{3}{2} + 2\cdot\frac{4}{3} + 2\cdot\frac{4}{4} + 5\cdot\frac{5}{6} + 1\cdot\frac{6}{9} = 11. \end{aligned}$$

As $ReZG_2(G) = \sum_{uv \in E(G)} \frac{d_u \cdot d_v}{d_u + d_v}$ and $ReZG_3(G) = \sum_{uv \in E(G)} (d_u \cdot d_v)(d_u + d_v)$, by using the similar methods we get the results. □

Theorem 2.7. *The reformulated Zagreb indices of dopamine are* $RM_1(C_8H_{11}NO_2) = 78$ *and* $RM_2(C_8H_{11}NO_2) = 108$.

Proof. In $C_8H_{11}NO_2$, the degrees of the edges $d(uv)$ where uv is an edge are 1, 2, 3 and 4. The number of these edge degrees of dopamin are $\mid d(uv) = 1 \mid = 1, \mid d(uv) = 2 \mid = 4, \mid d(uv) = 3 \mid = 5$ and $\mid d(uv) = 4 \mid = 1$. We know that $RM_1(G) = \sum_{uv \in E(G)} d(uv)^2$, i.e.,

$$\begin{aligned} RM_1(C_8H_{11}NO_2) &= \mid d(uv) = 1 \mid \cdot 1^2 + \mid d(uv) = 2 \mid \cdot 2^2 + \mid d(uv) = 3 \mid \cdot 3^2 \\ &+ \mid d(uv) = 4 \mid \cdot 4^2 \\ &= 1\cdot 1^2 + 4\cdot 2^2 + 5\cdot 3^2 + 1\cdot 4^2 = 78. \end{aligned}$$

For calculating $RM_2(C_8H_{11}NO_2)$, we partition the incident edges of dopamine according to the product of their edge degrees $d(e)\cdot d(e')$ where $e, e' \in E$ and e e'. In $C_8H_{11}NO_2$, we get $d(1)\cdot d(2), d(2)\cdot d(3), d(2)\cdot d(4), d(3)\cdot d(3)$ and $d(3)\cdot d(4)$. The number of these type of products are 1, 5, 2, 4 and 2, respectively.

We know that $RM_2(G) = \sum_{e,e' \in E(G)} d(e)d(e')$, i.e.,

$$\begin{aligned} RM_2(C_8H_{11}NO_2) &= \mid d(1)\cdot d(2) \mid \cdot 1\cdot 2 + \mid d(2)\cdot d(3) \mid \cdot 2\cdot 3 + \\ &+ \mid d(2)\cdot d(4) \mid \cdot 2\cdot 4 + \mid d(3)\cdot d(3) \mid \cdot 3\cdot 3 + \\ &+ \mid d(3)\cdot d(4) \mid \cdot 3\cdot 4 \\ &= 1\cdot 2 + 5\cdot 6 + 2\cdot 8 + 4\cdot 9 + 2\cdot 12 = 108. \end{aligned}$$

□

Theorem 2.8. *The reformulated F-index of dopamine is* $RF(C_8H_{11}NO_2) = 232$.

Proof. We know that $RF(G) = \sum_{uv \in E(G)} d(uv)^3$, i.e.,

$$\begin{aligned} RF(C_8H_{11}NO_2) &= \mid d(uv) = 1 \mid \cdot 1^3 + \mid d(uv) = 2 \mid \cdot 2^3 + \mid d(uv) = 3 \mid \cdot 3^3 \\ &+ \mid d(uv) = 4 \mid \cdot 4^3 \\ &= 1 \cdot 1^3 + 4 \cdot 2^3 + 5 \cdot 3^3 + 1 \cdot 4^3 = 232. \end{aligned}$$

□

Theorem 2.9. *The Banhatti indices of dopamine are* $B_1(C_8H_{11}NO_2) = 106$ *and* $B_2(C_8H_{11}NO_2) = 134$.

Proof. We know that $B_1(G) = \sum_{u,e} d_G(u) + d(e)$, i.e.,

$$\begin{aligned} B_1(C_8H_{11}NO_2) &= 2[(2+1)+(2+3)] + 5[(2+3)+(3+3)] + \\ &+ [(4+3)+(4+3)] + 2[(2+2)+(2+2)] + \\ &+ (1+1)+(1+2) \\ &= 106. \end{aligned}$$

and

$$\begin{aligned} B_2(C_8H_{11}NO_2) &= 2[2 \cdot 1 + 2 \cdot 3] + 5[2 \cdot 3 + 3 \cdot 3] + [4 \cdot 3 + 4 \cdot 3] \\ &+ 2[2 \cdot 2 + 2 \cdot 2] + 1 \cdot 1 + 1 \cdot 2 \\ &= 134. \end{aligned}$$

□

Theorem 2.10. *The leap Zagreb indices of dopamine are* $LM_1(C_8H_{11}NO_2) = 68$, $LM_2(C_8H_{11}NO_2) = 73$ *and* $LM_3(C_8H_{11}NO_2) = 56$.

Proof. We know that $LM_1(G) = \sum_{u \in V(G)} d_2(u)^2$ and $LM_2(G) = \sum_{uv \in E(G)} d(u)d_2(v)$, i.e.,

$$\begin{aligned} LM_1(C_8H_{11}NO_2) &= 2 \cdot 1^2 + 3 \cdot 2^2 + 6 \cdot 3^2 \\ &= 68. \end{aligned}$$

and

$$LM_2(C_8H_{11}NO_2) = 4(2 \cdot 3) + 5(3 \cdot 3) + 3 \cdot 1 + 1 \cdot 1 = 73.$$

As $LM_3(G) = \sum_{u \in V(G)} d(u)d_2(u)$ by using the similar methods we get the results. □

3. **Conclusions**

As dopamine is synthesized in the brain and kidneys and as in popular belief, it is a source of pleasure and happiness many researchers have studied properties of dopamine. In this paper, we calculate some topological indices of one of the chemical compounds called dopamine. In the literature, there has been a large number of papers related to properties of similar chemical compounds, but there is no mathematical or chemical research on dopamine in similar sense. Therefore the results obtained in this paper are the first

ones and will be followed by other research papers.

References

[1] S. Fahn, *The history of dopamine and levodopa in the treatment of Parkinson's disease*, Movement Disorders **23 (3)**, 497508, 2008.

[2] F. M Benes, *Carlsson and the discovery of dopamine*, Trends in Pharmacological Sciences **22 (1)**, 4647, 2001.

[3] I. Gutman, N. Trinajstic, *Graph theory and molecular orbitals III. Total π-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17**, 535-538, 1972.

[4] H. Aram, N. Dehgardi, *Reformulated F-index of graph operations*, Commun. Comb. Optim. **2**, 87-98, 2017.

[5] K. C. Das, N. Akgunes, M. Togan, A. Yurttas, I. N. Cangul, A. S. Cevik, *On the first Zagreb index and multiplicative Zagreb coindices of graphs*, Analele Stiintifice ale Universitatii Ovidius Constanta **24 (1)**, 153-176, 2016.

[6] K. C. Das, A. Yurttas, M. Togan, I. N. Cangul, A. S. Cevik, *The multiplicative Zagreb indices of graph operations*, Journal of Inequalities and Applications **90**, 2013.

[7] P. S. Ranjini, V. Lokesha, A. Usha, *Relation between phenylene and hexagonal squeeze using harmonic index*, Int. J. of Graph Theory **1**, 116-121, 2013.

[8] B. Furtula, I. Gutman, *A Forgotten Topological Index*, J. Math. Chem. **53 (4)**, 1184-1190, 2015.

[9] L. Zhong, *The harmonic index on graphs*, Applied Mathematics Letters **25**, 561-566, 2012.

[10] A. Milievi, S. Nikoli, N. Trinajsti, *On reformulated Zagreb indices*, Mol. Divers. **8**, 393399, 2004.

[11] I. Gutman, N. Trinajstic, *Graph Theory and Molecular Orbitals. Total pi electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17**, 535-538, 1972.

[12] V. R. Kulli, *On K Banhatti indices of graphs*, J. Comput. Math. Sci. **7**, 213218, 2016.

[13] B. Furtula, A. Graovac, D. Vukicevic, *Augmented Zagreb Index*, Journal of Mathematical Chemistry **48**, 370-380, 2010.

(First Author) Faculty of Arts and Science Department of Mathematics Uludag University 16059 Bursa, TURKEY.

E-mail address: ayurttas@uludag.edu.tr